Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2026 – 02:07 PM EST

PDB ID	:	9OVG / pdb_00009ovg
Title	:	Crystal Structure of Human Estrogen Receptor-alpha (Y537S) in complex with NCOA2 peptide and (E)-7-(4-hydroxystyryl)-2,2-dimethyl-6-(3-methylbut-2-en-1-yl)chroman-5-ol
Authors	:	Nwachukwu, J.C.; Chittiboyina, A.G.; Izard, T.; Nettles, K.W.
Deposited on	:	2025-05-30
Resolution	:	2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

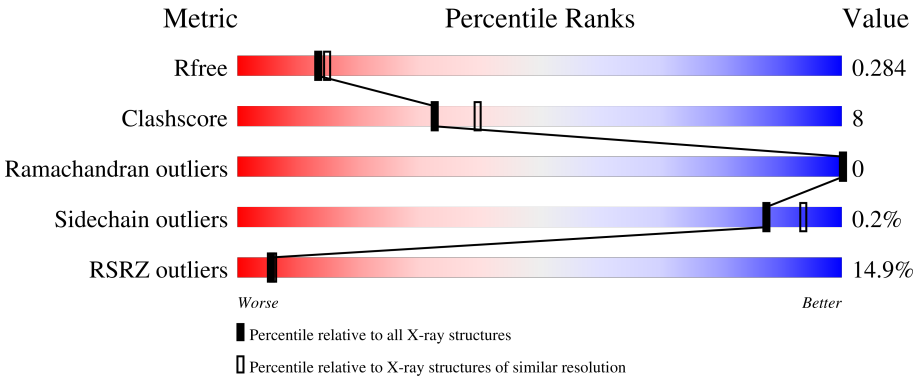
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	14% 75% 16% 9%
1	B	258	13% 70% 21% 9%
2	C	13	31% 62% 8% 31%
2	D	13	38% 31% 31%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	602	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3931 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	236	Total	C	N	O	S	0	0	0
			1850	1185	319	328	18			
1	A	236	Total	C	N	O	S	0	0	0
			1844	1180	319	327	18			

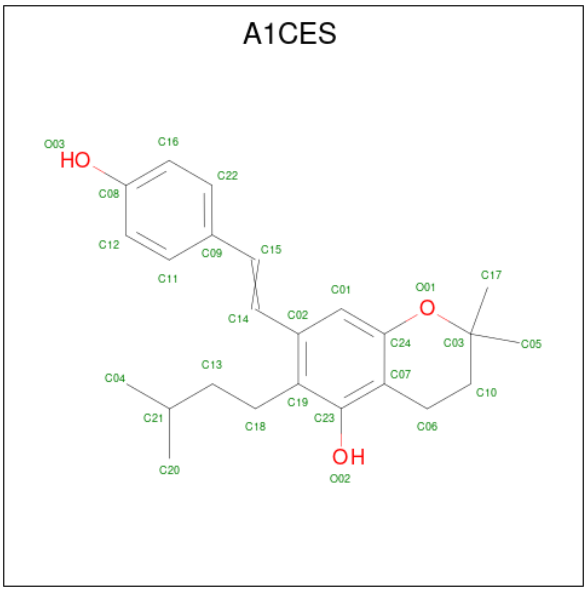
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	537	SER	TYR	engineered mutation	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			79	51	16	12			
2	D	9	Total	C	N	O	0	0	0
			79	51	16	12			

- Molecule 3 is 7-[2-(4-hydroxyphenyl)ethyl]-2,2-dimethyl-6-(3-methylbutyl)-3,4-dihydro-2H-1-benzopyran-5-ol (CCD ID: A1CES) (formula: $C_{24}H_{30}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 27 24 3	0	0
3	A	1	Total C O 27 24 3	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

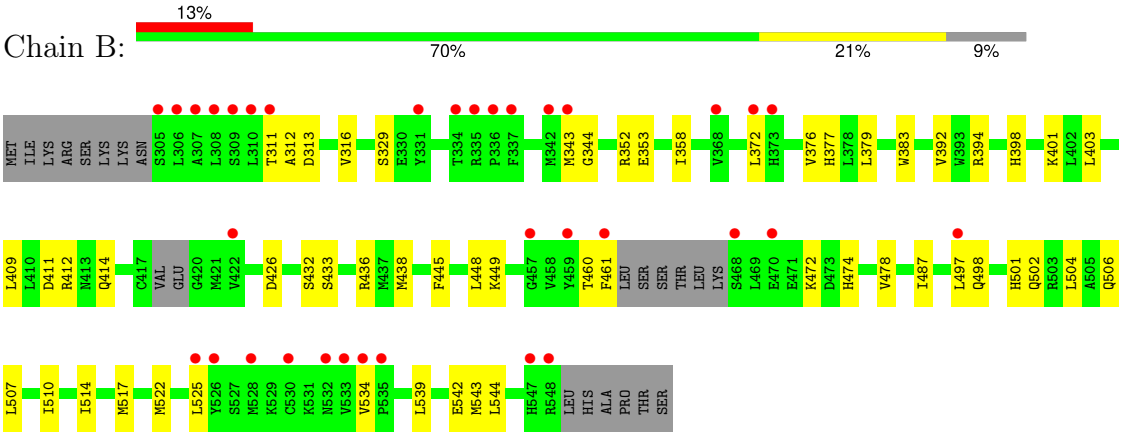
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	8	Total O 8 8	0	0
5	A	16	Total O 16 16	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

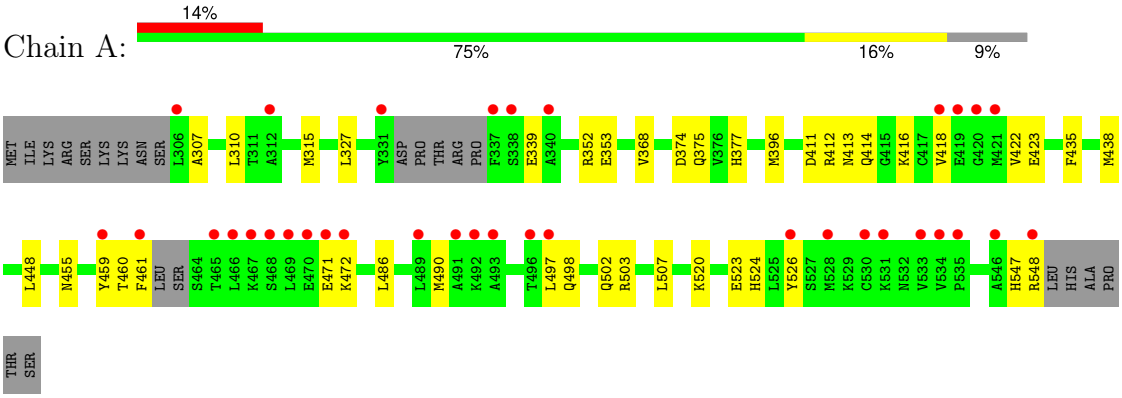
• Molecule 1: Estrogen receptor

Chain B:



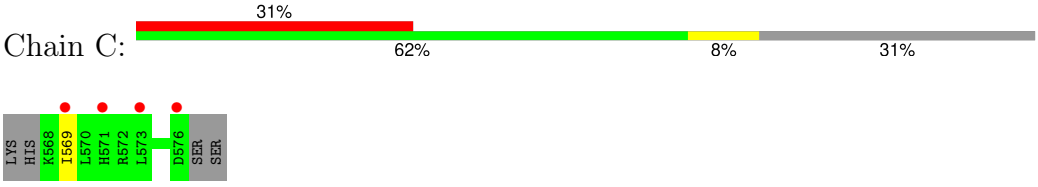
• Molecule 1: Estrogen receptor

Chain A:



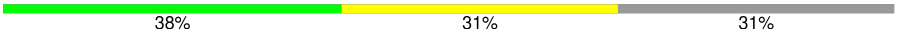
• Molecule 2: Nuclear receptor coactivator 2

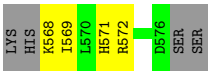
Chain C:



• Molecule 2: Nuclear receptor coactivator 2

Chain D:




LYS
HIS
K568
I569
L570
H571
R572
D576
SER
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.07Å 82.42Å 58.52Å 90.00° 110.87° 90.00°	Depositor
Resolution (Å)	54.68 – 2.28 54.68 – 2.28	Depositor EDS
% Data completeness (in resolution range)	57.4 (54.68-2.28) 57.5 (54.68-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.21	Depositor
R, R_{free}	0.225 , 0.286 0.225 , 0.284	Depositor DCC
R_{free} test set	664 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3931	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1CES, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.16	0/1875	0.33	0/2534
1	B	0.13	0/1884	0.31	0/2548
2	C	0.14	0/79	0.44	0/104
2	D	0.16	0/79	0.36	0/104
All	All	0.15	0/3917	0.32	0/5290

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1844	0	1861	27	0
1	B	1850	0	1874	33	0
2	C	79	0	88	1	0
2	D	79	0	88	2	0
3	A	27	0	0	0	0
3	B	27	0	0	1	0
4	A	1	0	0	2	0
5	A	16	0	0	1	0
5	B	8	0	0	0	0
All	All	3931	0	3911	62	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:LEU:HD21	1:A:497:LEU:HD21	1.65	0.79
1:A:486:LEU:O	1:A:490:MET:HG3	1.83	0.78
1:A:411:ASP:OD2	1:A:412:ARG:N	2.26	0.67
1:A:490:MET:HE1	1:A:503:ARG:HB3	1.77	0.66
1:B:448:LEU:HD11	1:B:507:LEU:HD22	1.79	0.65
1:A:448:LEU:HD11	1:A:507:LEU:HD22	1.80	0.64
1:B:411:ASP:HB3	1:B:414:GLN:HG3	1.80	0.63
1:B:498:GLN:HA	1:B:501:HIS:CE1	2.34	0.63
1:A:438:MET:O	1:A:503:ARG:NH1	2.28	0.62
1:B:474:HIS:O	1:B:478:VAL:HG23	2.03	0.58
1:A:339:GLU:HG3	1:A:418:VAL:HG12	1.86	0.57
1:B:514:ILE:HA	1:B:517:MET:HE2	1.88	0.56
1:A:423:GLU:H	1:A:423:GLU:CD	2.14	0.56
1:B:377:HIS:NE2	1:B:460:THR:HB	2.22	0.55
1:B:343:MET:HB3	1:B:534:VAL:HG21	1.89	0.53
1:A:520:LYS:O	1:A:523:GLU:HG2	2.09	0.52
1:A:416:LYS:HA	1:A:422:VAL:HG22	1.92	0.52
1:B:372:LEU:O	1:B:376:VAL:HG23	2.10	0.51
4:A:602:CL:CL	5:A:714:HOH:O	2.57	0.51
1:B:313:ASP:HA	1:B:316:VAL:HG12	1.93	0.50
1:A:411:ASP:H	1:A:414:GLN:HG3	1.78	0.49
1:A:411:ASP:HB3	1:A:413:ASN:OD1	2.13	0.49
1:B:506:GLN:O	1:B:510:ILE:HG12	2.13	0.49
1:A:307:ALA:HA	1:A:310:LEU:HD12	1.95	0.49
1:B:539:LEU:O	1:B:543:MET:HG2	2.13	0.48
1:A:498:GLN:O	1:A:502:GLN:HG3	2.14	0.48
1:A:461:PHE:HB2	1:A:472:LYS:HE3	1.96	0.47
1:A:377:HIS:NE2	1:A:460:THR:HB	2.28	0.47
1:B:329:SER:HA	1:B:352:ARG:HH22	1.79	0.47
1:B:411:ASP:OD1	1:B:412:ARG:N	2.48	0.46
1:B:438:MET:HE1	1:B:507:LEU:HD23	1.97	0.46
2:D:569:ILE:HG23	2:D:572:ARG:NH2	2.31	0.46
1:B:502:GLN:O	1:B:506:GLN:HG2	2.17	0.45
1:A:327:LEU:HD12	1:A:353:GLU:HG2	1.98	0.45
1:B:412:ARG:NE	1:B:426:ASP:OD2	2.47	0.44
1:A:374:ASP:OD2	1:A:471:GLU:HG2	2.17	0.44
1:A:526:TYR:CE1	1:A:548:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:TRP:NE1	1:B:522:MET:HE1	2.33	0.44
1:B:433:SER:OG	1:B:436:ARG:NH2	2.50	0.44
1:B:358:ILE:HG13	1:B:379:LEU:HD13	2.00	0.44
1:B:394:ARG:HB3	1:B:403:LEU:HD23	2.01	0.43
1:B:392:VAL:HG13	1:B:432:SER:HA	2.00	0.43
1:B:542:GLU:CD	2:C:569:ILE:HG22	2.43	0.43
1:A:455:ASN:ND2	1:A:459:TYR:OH	2.47	0.43
1:B:311:THR:OG1	1:B:312:ALA:N	2.52	0.42
1:B:487:ILE:HD11	1:B:504:LEU:HD22	2.01	0.42
1:A:315:MET:HE2	1:A:315:MET:HB2	1.95	0.42
2:D:568:LYS:HB2	2:D:571:HIS:HD2	1.85	0.42
1:B:510:ILE:O	1:B:514:ILE:HG13	2.20	0.42
1:B:525:LEU:HG	1:B:544:LEU:HD11	2.02	0.42
1:B:344:GLY:HA2	1:B:534:VAL:HG11	2.03	0.41
1:A:352:ARG:HD2	4:A:602:CL:CL	2.57	0.41
1:A:411:ASP:OD2	1:A:412:ARG:HG2	2.20	0.41
1:B:353:GLU:OE1	3:B:601:A1CES:O03	2.39	0.41
1:B:398:HIS:CD2	1:B:409:LEU:HD11	2.55	0.41
1:B:401:LYS:HB3	1:B:409:LEU:CD2	2.50	0.41
1:B:461:PHE:HB2	1:B:472:LYS:HE2	2.03	0.41
1:B:445:PHE:CZ	1:B:449:LYS:HD3	2.56	0.40
1:A:396:MET:SD	1:A:435:PHE:HB3	2.60	0.40
1:A:368:VAL:HA	1:A:375:GLN:NE2	2.37	0.40
1:A:490:MET:HE2	1:A:490:MET:HB3	1.92	0.40
1:A:524:HIS:ND1	1:A:524:HIS:C	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	230/258 (89%)	225 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	230/258 (89%)	227 (99%)	3 (1%)	0	100	100
2	C	7/13 (54%)	7 (100%)	0	0	100	100
2	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	474/542 (88%)	466 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/233 (86%)	199 (100%)	1 (0%)	81	89
1	B	204/233 (88%)	204 (100%)	0	100	100
2	C	9/13 (69%)	9 (100%)	0	100	100
2	D	9/13 (69%)	9 (100%)	0	100	100
All	All	422/492 (86%)	421 (100%)	1 (0%)	87	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	356	HIS
1	B	373	HIS
1	B	375	GLN
1	B	398	HIS
1	B	413	ASN
1	B	439	ASN
1	B	506	GLN

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Mol	Chain	Res	Type
1	B	516	HIS
1	A	356	HIS
1	A	455	ASN
1	A	498	GLN
1	A	513	HIS
1	A	516	HIS
2	D	571	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	A1CES	B	601	-	29,29,29	2.69	15 (51%)	40,42,42	1.87	10 (25%)
3	A1CES	A	601	-	29,29,29	2.81	16 (55%)	40,42,42	1.89	8 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1CES	B	601	-	-	6/10/21/21	0/3/3/3
3	A1CES	A	601	-	-	5/10/21/21	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	A1CES	C02-C14	-7.52	1.35	1.47
3	B	601	A1CES	C02-C14	-7.30	1.35	1.47
3	A	601	A1CES	C02-C19	-4.77	1.36	1.40
3	B	601	A1CES	C02-C19	-4.69	1.36	1.40
3	B	601	A1CES	O01-C03	-4.53	1.39	1.46
3	A	601	A1CES	O01-C03	-4.40	1.39	1.46
3	A	601	A1CES	C09-C15	-4.38	1.35	1.47
3	B	601	A1CES	C09-C15	-4.28	1.35	1.47
3	A	601	A1CES	C24-C07	-4.10	1.34	1.40
3	A	601	A1CES	C01-C02	-3.81	1.34	1.40
3	B	601	A1CES	C01-C02	-3.77	1.34	1.40
3	A	601	A1CES	C23-C07	-3.76	1.34	1.40
3	B	601	A1CES	C24-C07	-3.64	1.34	1.40
3	A	601	A1CES	C23-C19	-3.44	1.35	1.40
3	B	601	A1CES	C23-C07	-3.31	1.35	1.40
3	A	601	A1CES	C01-C24	-3.03	1.33	1.38
3	B	601	A1CES	C23-C19	-3.00	1.35	1.40
3	B	601	A1CES	C01-C24	-2.78	1.34	1.38
3	A	601	A1CES	C12-C11	-2.77	1.34	1.38
3	B	601	A1CES	C16-C22	-2.73	1.34	1.38
3	A	601	A1CES	C13-C21	-2.70	1.34	1.51
3	B	601	A1CES	C13-C21	-2.66	1.34	1.51
3	A	601	A1CES	C16-C22	-2.62	1.34	1.38
3	B	601	A1CES	C12-C11	-2.49	1.34	1.38
3	A	601	A1CES	C12-C08	-2.39	1.34	1.39
3	B	601	A1CES	C12-C08	-2.24	1.34	1.39
3	B	601	A1CES	C16-C08	-2.23	1.34	1.39
3	A	601	A1CES	C11-C09	-2.21	1.35	1.39
3	A	601	A1CES	C16-C08	-2.18	1.34	1.39
3	B	601	A1CES	C11-C09	-2.07	1.35	1.39
3	A	601	A1CES	C22-C09	-2.00	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	A1CES	C24-C07-C23	4.78	122.57	117.49
3	B	601	A1CES	O01-C24-C07	4.72	125.50	122.53
3	B	601	A1CES	C01-C24-C07	-4.59	116.92	122.06
3	A	601	A1CES	C10-C06-C07	-4.59	103.94	111.74
3	A	601	A1CES	C01-C24-C07	-4.41	117.12	122.06
3	A	601	A1CES	C18-C13-C21	4.07	127.72	114.70
3	B	601	A1CES	C18-C13-C21	3.79	126.81	114.70
3	B	601	A1CES	C24-C07-C23	3.59	121.31	117.49
3	B	601	A1CES	C03-O01-C24	3.25	120.57	117.20
3	B	601	A1CES	C10-C06-C07	-3.06	106.54	111.74
3	A	601	A1CES	O01-C03-C10	2.57	111.90	108.87
3	B	601	A1CES	C20-C21-C13	2.39	125.72	111.55
3	B	601	A1CES	C02-C01-C24	2.35	124.49	120.74
3	B	601	A1CES	C01-C02-C19	-2.32	117.26	119.93
3	A	601	A1CES	C20-C21-C13	2.24	124.84	111.55
3	A	601	A1CES	C02-C19-C23	2.19	120.52	118.60
3	A	601	A1CES	C19-C23-C07	-2.12	118.64	122.31
3	B	601	A1CES	O01-C03-C10	2.10	111.35	108.87

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	A1CES	C02-C14-C15-C09
3	A	601	A1CES	C02-C14-C15-C09
3	B	601	A1CES	C21-C13-C18-C19
3	A	601	A1CES	C01-C02-C14-C15
3	A	601	A1CES	C19-C02-C14-C15
3	A	601	A1CES	C18-C13-C21-C20
3	B	601	A1CES	C18-C13-C21-C20
3	A	601	A1CES	C21-C13-C18-C19
3	B	601	A1CES	C18-C13-C21-C04
3	B	601	A1CES	C19-C02-C14-C15
3	B	601	A1CES	C01-C02-C14-C15

There are no ring outliers.

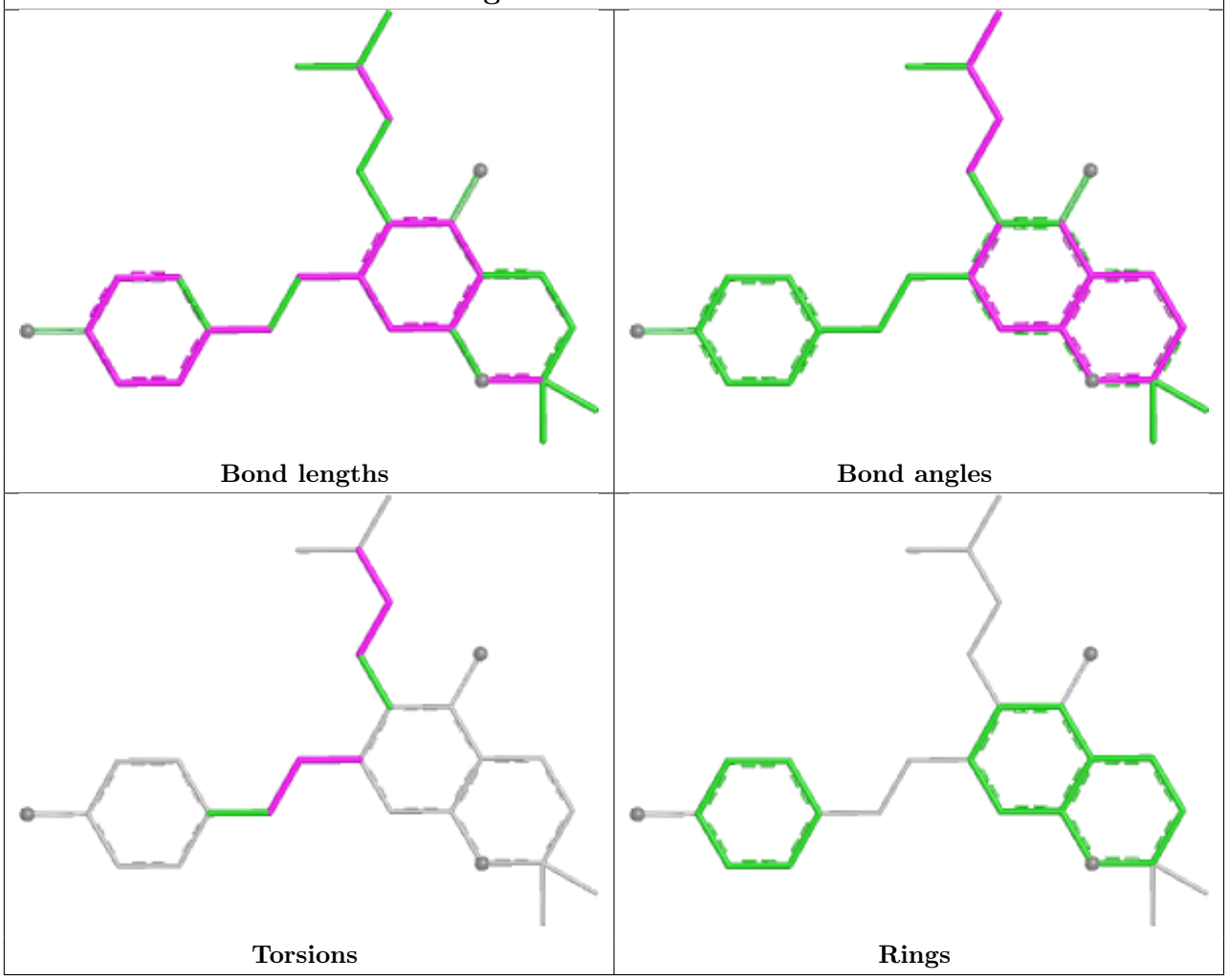
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	A1CES	1	0

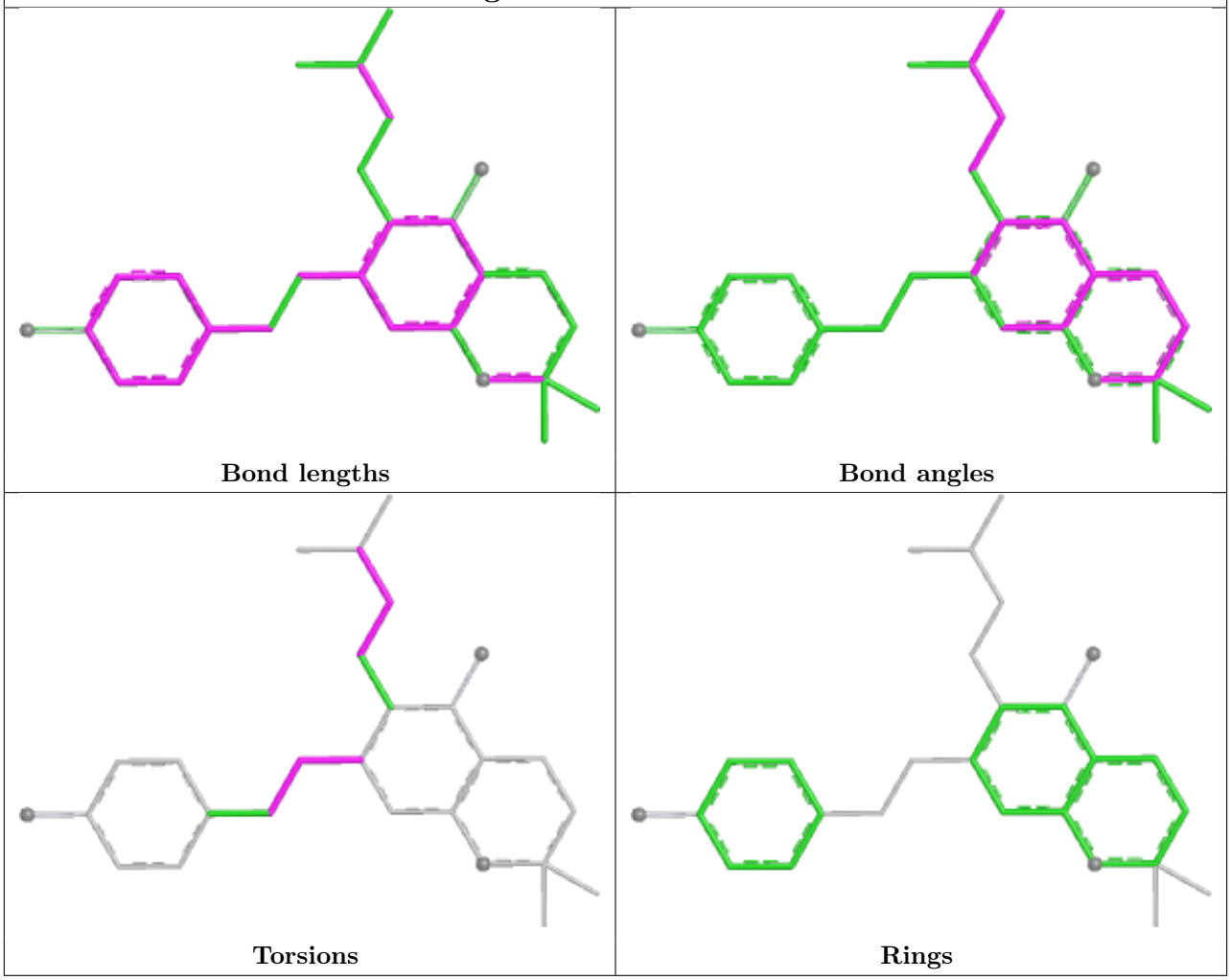
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1CES B 601



Ligand A1CES A 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	236/258 (91%)	0.86	35 (14%) 5 6	19, 44, 79, 87	0
1	B	236/258 (91%)	0.97	34 (14%) 6 6	23, 46, 83, 91	0
2	C	9/13 (69%)	1.63	4 (44%) 0 0	50, 62, 78, 81	0
2	D	9/13 (69%)	0.91	0 100 100	45, 46, 66, 70	0
All	All	490/542 (90%)	0.93	73 (14%) 5 6	19, 46, 81, 91	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	533	VAL	4.7
1	A	459	TYR	4.5
1	A	468	SER	4.0
1	B	535	PRO	4.0
1	B	525	LEU	3.9
1	B	337	PHE	3.8
1	A	306	LEU	3.8
1	A	534	VAL	3.8
1	A	492	LYS	3.6
1	B	526	TYR	3.6
1	A	337	PHE	3.6
1	B	308	LEU	3.6
1	B	336	PRO	3.6
1	A	420	GLY	3.5
1	A	470	GLU	3.5
1	B	470	GLU	3.4
1	A	471	GLU	3.4
1	A	469	LEU	3.3
1	B	534	VAL	3.3
1	B	335	ARG	3.3
1	B	547	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	3.2
1	B	306	LEU	3.2
1	A	466	LEU	3.2
1	A	491	ALA	3.1
1	B	331	TYR	3.1
1	B	497	LEU	3.1
1	B	307	ALA	3.1
1	A	493	ALA	3.1
1	A	530	CYS	3.1
1	B	528	MET	2.9
1	A	461	PHE	2.9
1	B	468	SER	2.8
1	B	459	TYR	2.8
1	A	526	TYR	2.7
1	A	418	VAL	2.6
1	A	472	LYS	2.6
1	A	535	PRO	2.6
1	B	373	HIS	2.6
1	A	533	VAL	2.6
1	A	467	LYS	2.6
1	B	530	CYS	2.5
1	A	528	MET	2.5
1	A	465	THR	2.5
2	C	569	ILE	2.5
2	C	571	HIS	2.5
1	B	548	ARG	2.5
1	B	311	THR	2.4
1	B	343	MET	2.4
1	A	546	ALA	2.4
2	C	573	LEU	2.4
1	B	305	SER	2.3
1	B	309	SER	2.3
1	B	368	VAL	2.3
1	A	497	LEU	2.3
1	A	419	GLU	2.3
1	A	338	SER	2.3
1	A	331	TYR	2.3
1	A	548	ARG	2.3
1	A	531	LYS	2.3
1	A	312	ALA	2.3
1	B	342	MET	2.2
1	A	489	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	334	THR	2.2
1	A	340	ALA	2.2
1	B	461	PHE	2.2
1	B	532	ASN	2.1
1	B	457	GLY	2.1
1	A	421	MET	2.1
1	B	372	LEU	2.1
1	B	422	VAL	2.1
1	A	496	THR	2.0
2	C	576	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

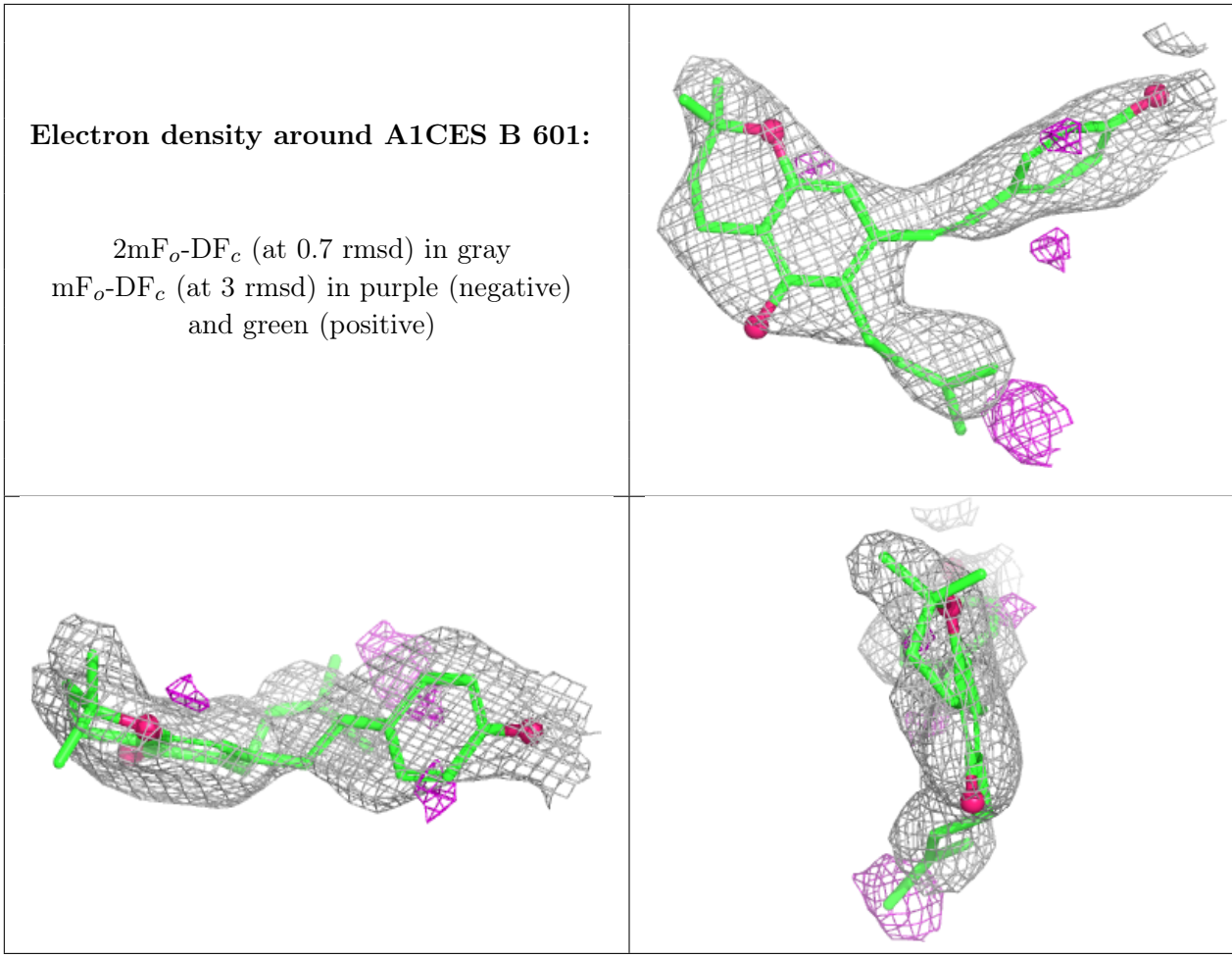
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	A1CES	B	601	27/27	0.81	0.17	26,60,75,84	0
3	A1CES	A	601	27/27	0.87	0.14	28,49,80,85	0
4	CL	A	602	1/1	0.96	0.07	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

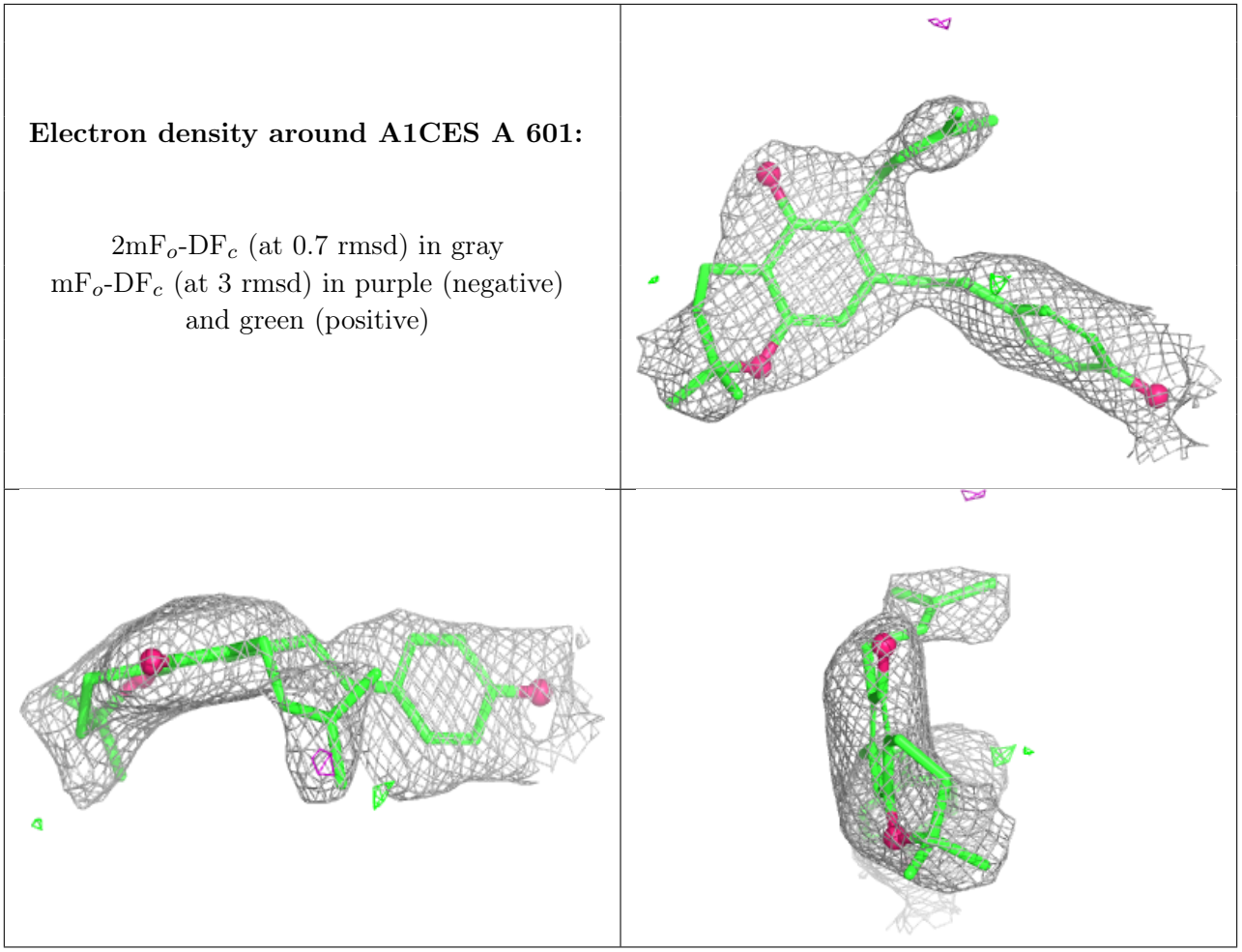
Electron density around A1CES B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1CES A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.